

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 59.1 °C

Global applicability domain: Inside

Local applicability domain index: 3.27e-01

Confidence level: 3.61e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Monocrotophos</div> <div>Measured: 55.0</div> <div>Predicted: 59.1</div>	<div>Image not found</div> <div>Omethoate</div> <div>Measured: -28.0</div> <div>Predicted: -10.2</div>	<div>Image not found</div> <div>Diethyl formamidomalonate</div> <div>Measured: 48.5</div> <div>Predicted: 65.3</div>
<div>Image not found</div> <div>Dimethoate</div> <div>Measured: 52.0</div> <div>Predicted: 43.1</div>	<div>Image not found</div> <div>4-Morpholinepropanesulfonic acid</div> <div>Measured: 284</div> <div>Predicted: 249</div>	